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ABSTRACT

The study of chemistry includes many abstract concepts that students may find difficult to understand. A fundamental yet troublesome part of introductory chemistry courses is the topic of electron configuration and specifically quantum-mechanical orbitals. In an effort to examine the way students internalize the concept of atomic orbitals and how they attempt to communicate that understanding using models, a study was undertaken. First, a pilot study was conducted with 20 college students in a teacher training program in order to identify specific misunderstandings related to a scientific conception of orbitals. These students were asked a single question: "If you had to explain the concept of orbitals to students in a chemistry course, how would you do so?" From the responses, three modes of communication emerged: written descriptions, symbolic representations, and pictorial approaches. The pilot study served as a basis to construct research questions for a survey of 302 grade 12 chemistry students and students in a university introductory chemistry course to determine students' use of the three communication styles. Findings suggest that many students have trouble with the symbolic conventions of electron configuration. The use of appropriate models to explain orbitals is suggested. (Contains 31 references.) (WRM)

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Students' Understanding of Orbitals: A Survey

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Introduction

Science in general and specifically chemistry have their share of abstract concepts. A fundamental part of introductory chemistry education is the building of the concept of electron configuration which necessitates a discussion of orbitals. Students have traditionally found this topic particularly difficult to understand. The source of this difficulty has been alluded to by chemical educators for at least twenty years. Herron (1975), Bent (1984) and Beistel (1975) have suggested that many of our high school chemistry students are working at what Piaget would refer to as a concrete operational cognitive level. This would imply that students require significant concrete modeling of concepts yet many introductory chemistry textbooks begin with a study of " . . . the nature of atoms (which is decidedly not concrete) . . ." (Herron, 1975). The need for adequate modeling has been further supported by the work of Gardner (1983) which emphasizes the variety of student learning styles which he frames as multiple intelligences. To name a few, Barnea (1995), Gillespie (1995), Streitberger (1994) and Zeigler (1996) have provided pedagogical support for this perceived need to incorporate models in chemistry instruction.

Although there has been some research (e.g., Siemankowski & MacKnight, 1971; Talley, 1973) to suggest a link between use of physical models and improved assessed performance, there remains an abundance of literature which identifies students' misconceptions in chemistry education. These misconceptions as defined by Fisher (1985) have been the subject of much study (e.g., Duncan & Johnstone, 1979; Andersson, 1986; Peterson, Treagust & Garnett, 1989; BouJaoude, 1991; Schmidt, 1992; Griffiths & Preston, 1992; Staver & Lumpe, 1995) and are invariably associated with pedagogical use of models or lack thereof.

This may be a clue that though models are being used they are having varying impact. A survey of model usage impact on grade seven and eleven science students (Grosslight, Unger, Jay & Smith, 1991) has identified three levels of student understanding concerning the rationale behind using models in science instruction. Students with a viewpoint at level one " . . . think of models as little copies of real-world objects." (Grosslight et al., 1991). Students who have adopted a level two understanding " . . . realize that there is a specific explicit purpose that mediates the way the model is constructed. . . . tests of the model are not thought of as tests of underlying ideas but of the workability of the model itself."(Grosslight et al.). With a level three viewpoint a student appreciates that a model allows for at least the following three criteria to be met:

> First, the model is now constructed in the service of developing and testing ideas rather than as serving as a copy of reality itself. Second, the modeler takes an active role in constructing the model, evaluating which of several models could be used to serve the model's purpose. Third, models can be manipulated and subjected to tests in the service of informing ideas. Thus, they provide information within a cyclic constructive process. (Grosslight et al.)

If the justification and application framework for using models in science has been clearly defined for educators then it should be evident in the ease with which students communicate their ideas using models.

In an effort to examine the way students internalize the concept of atomic orbitals and perhaps more importantly how they attempt to communicate that understanding using models, the following study was undertaken.

Pilot Study

In order to identify specific misunderstandings en route to a conception of orbitals, a pilot study was conducted with twenty college students in a teacher-training program. These students had completed a high school chemistry core (i.e., two courses, grade 11 and 12) some time in the past four years. In a taped interview, the students were asked a single question. If you had to explain the concept of orbitals to a student in a chemistry course, how would you do so? From transcriptions of these interviews and associated notes and diagrams made by students, three modes of communication emerged: written descriptions (e.g., definitions, conventions and explanations), symbolic representations (e.g., electron configurations, dot diagrams and orbital notations) and pictorial approaches (e.g., stick and projectional drawings).

The pilot study served as a basis to construct research questions.

Specific Research Goals

The following questions represent the primary research interest:

1. Do students have a conception of orbitals that goes beyond a purely symbolic representation?

2. To what extent has the student's spatial concept of orbitals been developed?

3. What types of modeling have instructors incorporated to facilitate students' constructing of meaning?

4. Are students able to apply an orbital concept in explaining observed bonding trends?

5. At what stage of their conceptual restructuring do students tend to encounter the most difficulty?

Methods

A pencil and paper survey was designed to probe students' relative use of the following response styles: symbolic (recall), written (low level understanding), pictorial representations, integrated application / explanation and model usage.

Internal validity was judged by applying the survey to two independent groups of ten first year university science students. Following each of three trials on successive new groups, the survey was refined as per suggestions of independent chemistry instructors.

The sample (n=302) consisted of students in the first semester of grade twelve chemistry and students in the first semester of introductory chemistry at university. This group was chosen based on completion of at least a first course in chemistry where the bulk of orbital theory tends to be introduced in many schools.

Some questions tended to be open-ended by design for two reasons: to allow students to communicate their response using representations most comfortable to them and to avoid cueing effects (i.e. "Oh I remember this *type* of question!").

External validity was promoted by a random sampling of students from across Canada. Post-secondary students surveyed were from universities in Nova Scotia, Newfoundland, Ontario and Alberta . High school students surveyed were attending schools in New Brunswick, Nova Scotia, Alberta, Newfoundland and Ontario. Approximately equal numbers of students represented each of the groups (i.e., university/high school students) and subgroups (i.e., provincial).

Reliability was assessed by the following means:

1. A test-retest on a pilot group of twenty students with one week separation between tests and no direct intermediary instruction yielded a correlation coefficient of 0.90.

2. Interscorer reliability was undertaken on twenty surveys (three markers) and generated a correlation coefficient of 0.88.

3. Internal consistency reliability indicated an alpha coefficient of 0.74 , a mean index of difficulty = 0.55 and a mean index of discrimination = 0.52 . These values have limited implication considering the nature of some of the questions in the survey.

The Survey/Analysis

Chemistry instructors were told to distribute the survey randomly to their students. Other materials included a supplied periodic chart showing only symbols, atomic numbers and atomic masses and examination foolscap. Students were to be given unlimited time to complete the survey on the supplied paper under instructor supervision. The survey questions and analysis of responses follows. All percentages quoted with respect to students responses are based on n=302.

1. Give the electron configuration for $_{35}Br$.

Only 36% of respondents were able to give the correct electron configuration despite having been supplied with a periodic table. Of the incorrect answers a pattern of two groups emerged. A considerable number of students were confused over the terminology and supplied a variety of answers including electron totals, dot pictures, unlabelled concentric circle models and unlabelled orbital notations. A second group included those who provided a configuration which reflected a miss ordering of the "d" orbital (i.e., ... 4s, 4d, 4p). From drawings adjacent to many of their answers, it was obvious that students were making use of a familiar (e.g., Tzimopoulos, Metcalfe, Williams & Castka, 1978, p. 115; McQuarrie & Rock, 1991, p. 328) snake-like ordering chart to generate a configuration.

2. In using a conventional representation $1s^2$, what does each of the symbols represent?

a. The number 1 represents ...

b. The letter "s" represents ...

c. The superscript "2" represents ...

Correct answers accounted for 46%, 60% and 58% respectively of the total number of students surveyed. In part "a", students responding incorrectly frequently considered a shell to be synonymous with an orbital. Again in part "b" the letter "s" was incorrectly considered to be a shell type. Incorrect answers in part "c" were split between numbers of electrons in the shell and numbers of valence electrons. Correct responses in some cases encompassed a purely quantum mechanical approach and a strongly mathematical justification. This very theoretical slant at times seemed to amount to rote response though this was difficult to judge. Confusion in terminology continued to be a prominent pattern in this question of symbolic nature.

3. How many valence electrons does bromine have?

Considering the difficulty students encountered with earlier questions, it was not surprising to find that only 58% of students were able to respond correctly. This question was particularly demonstrative in the failed responses. Popular incorrect answers in order of decreasing occurrence included, one valence electron (likely a reversal on the octet rule), five valence electrons (perhaps a misunderstanding that the valence shell includes 4s electrons), seventeen valence electrons (most probably inclusion of the 3d electrons as part of the n= shell) and lastly thirty-five electrons (which represents total electrons). One apparent misunderstanding that students have is the placement of the "d" orbitals with respect to "s" and "p" orbitals of similar energy. In dealing with "d" orbitals, instructors would do well to explain the placement of 3d adjacent to 4s in terms of distance from the nucleus, energy of electrons and the spatial relationship within the n=4 shell.

4. What is the anticipated charge on a bromine ion and how do you account for such a charge?

Eighty-five percent of students were able to designate a likely charge of -1 on bromine ion. Only 40% of students were able to account for the charge using an octet stability argument. Among less complete answers the most popular (20%) was a proton-electron tally. A popular response to this question was to use the location of bromine in the periodic chart as the "reason" for the predicted charge. This may suggest that these students don't understand how chemical properties dictated the placement of elements in the periodic table and that these properties are directly related to electronic behaviors. This type of "retro-reasoning" using the periodic chart was also common in responses to other questions in the survey. The implication may be that students' understanding is limited to rote learning of patterns in the periodic table.

5. In your own words, describe what an orbital is.

Responses to this question were grouped. About one-third of students represented an orbital as a three-dimensional space and incorporated the idea of a probability map. Those recognizing the spatial component but neglecting the probability factor amounted to 26%. The theory that electrons travel in planar two-dimensional orbits that never change was held by 28% of students surveyed. The remaining responses were divided between totally incorrect answers and no answer supplied.

The existence of the two-dimensional conception of an orbital may arise from an extension of the Bohr model or possibly the frequently used analogy of planetary orbits. Over 10% of students went so far as to suggest that all multi-electron orbits are concentric despite the fact that they have no doubt been exposed to the idea of s, p, and d orbitals; all with very different shapes!

6. When we add electrons to orbitals sequentially in building up a model for a particular atom, what determines the ordering of orbitals?

Many of the students who gave an electron configuration for bromine were unable to provide the reasoning requested in this question. Of those surveyed, 27% made mention of energy as a factor. An attempt was made by 3% of students to explain the relationship between energy and distance from the nucleus. What consistently did arise was an Aufbau "building up" approach using the aforementioned orbital-ordering chart. Other responses showed sporadic understanding of orbital capacity, Hund's rule and the Pauli exclusion principle. It might be argued that these are part of a complete answer. A more specific question was avoided so as to preclude the cueing effect noted earlier.

7. How would you define a shell in the context of electron configuration?

Confusion in terminology was evident in the responses with only 25% of students able to correctly define a shell. The majority of answers were more from a descriptive quantum mechanical approach than a spatial perspective. The two most common incorrect answers involved confusion with an orbital and suggesting that a shell be only a term used in conjunction with valence electrons.

8. Why do elements in the same group of the periodic table often have similar properties?

Sixty-two percent of students indicated that the equal number of valence electrons was the key to this question. Incorrect answers included the same size, identical configuration, identical charge and common group!

9. Sketch a single picture of two different orbitals in the same shell.

The purpose of this question was to assess students' understanding of an orbital's orientation in space relative to other orbitals. A single picture of a px, py and pz orbitals represented 26% of responses. Nearly 40% drew an s and p type orbital confined by a boundary representing a shell. The outer limits of these orbitals touched the boundary of the shell.

10. Sketch and label a picture of how polar covalent bonding might occur between orbitals on the atoms hydrogen and chlorine in forming hydrogen chloride.

Answers were grouped as follows. Four percent of students sketched and labeled the overlapping orbitals 1s and 3p. Those that sketched an overlapping s and p orbital with no labels accounted for 6% of the total number surveyed. The largest group (31%) represented the bonding using a dot diagram with no particular labeling of orbitals. The remaining students gave incorrect answers or no answer to this question. Of the alternate conceptions two were prevalent a diagram of two overlapping circles with electrons shared and a dot diagram showing an ionic-like model of transferred electrons. It would seem that the idea of shared electrons is entrenched yet the orbitals used or the spatial nature of the overlap is beyond the students' expression. There was no evidence that students understood the rationale for a "polar" bond though this was not specifically asked for.

11. Draw an electron dot diagram for NH_3.

Many students (75%) represented bonding in ammonia using a dot diagram. The predominant oversight was the nitrogen lone pair.

12. The VSEPR theory is often used for predicting shapes of molecules. On what does this theory base its predictions?

One third of students answered that electron repulsion formed the basis for predicting shape. Another one third of students said that the common (e.g., Brady & Holum, 1993, p. 257; Atkins & Beran, 1990, p. 306; Tzimopoulos et al., 1978, p. 183) lone pair-bonding pair table and its corresponding electrons were the "reason" for the predicted shape. The final third answered incorrectly (no apparent pattern) or didn't supply an answer.

13. Sketch a picture of what you might expect NH_3 to look like based on the VSEPR theory.

This question presumes an understanding of VSEPR. A trigonal pyramidal shape was sketched by 22% of respondents. The most prevalent incorrect shape was a trigonal planar structure which may indicate two possible scenarios: students simply guessed at the structure using the formula and little knowledge of VSEPR or an incorrect application of VSEPR having neglected the effect of the lone pair on nitrogen.

14. A concept known as "hybridization" proposes that orbitals be mixed in certain proportions (i.e. sp, sp^2, sp^3).

a. Why do you think chemists needed to develop such an idea?

b. With the aid of a picture, explain what is meant by mixing orbitals.

Nearly one quarter of students suggested that bonding properties/lengths could not be accounted for by traditional orbital ideas and thus a hybridization concept was forwarded. Sixteen percent of students drew a picture of some type of sp mixing to form a hybrid orbital. These questions elicited few responses however; they addressed a topic that 20 % of students claimed was not covered in their grade eleven or twelve curriculum.

15. Using your choice of representations, describe fully the bonding you might expect in methane (CH_4).

Responses were grouped in the following manner: 27% used an electron dot picture as part of their answer, 29% used a line drawing with no perspective as part of their answer, 10% drew a tetrahedron using the wedge convention as part of their answer, 6% labeled orbitals and mentioned hybridization as part of their answer and 41% described the bonding in terms of covalent sharing as part of their answer.

16. Describe how orbitals have been modeled for you by your teachers. What types of visual aids have been used to enhance your spatial concept of orbitals?

Seventy percent of students noted that two-dimensional pictures from books, overheads and chalkboards were among their visual aids. Thirty percent of students had been taught using stick and ball models/kits as part of instruction. Twenty percent remembered having been taught with balloons. Ten percent made reference to a variety of analogies. Lastly two percent of students had access to computer simulation or calculation software.

Coverage in The Curriculum

Students in responding to questions in the survey were told to indicate if the question seemed to fall outside of the curriculum they had studied. Students highlighted the following areas as weaknesses in their curriculum background:

a. 10 % were unfamiliar with the term electron configuration.

b. 10 % were unfamiliar with the reasoning behind the orbital filling order.

c. 10% were unfamiliar with the shell concept.

d. 6% were unfamiliar with VSEPR theory.

e. 20% were unfamiliar with hybridization.

These figures, if accurate, may indicate some lack of coverage of topics. It would seem that much of the survey concerns itself with topics students should be aware of.

High School versus University Students

One may anticipate that since university students were further removed from their first chemistry course they may well have forgotten much of the theory especially by comparison to students who are still in high school. An attempt to compare performance of those currently enrolled in a second high school chemistry course and first year university science students as a whole, revealed no obvious trends. A difference may not be evident because of the diversity of backgrounds introduced into a university in the first year programs. There were individual high schools and universities which performed much better in certain areas but a curricular or pedagogical comparison was beyond the scope of this study.

Discussion/Implications

From this study it appears as though many students have difficulty with the symbolic conventions of electron configuration. In the first instance chemistry educators may attribute this lack of success in writing electron configurations as a matter of practice. The basis for "building up" a configuration and how it relates to patterns in the periodic table seems to be overshadowed by a myriad of memory aids. This may produce students who can recall quickly but it doesn't model the type of intuitive understanding we wish to cultivate in future chemists. Approaches (e.g., Atkins et al., 1990, p. 250 ; Brady et al., 1993, p. 193) which start with students recognizing patterns in the periodic table on their own and the teacher supporting these discoveries with the models and theory can prove to be much more effective than rote learning of orbital sequences.

As alluded to earlier, in recognizing questions, students have trouble distinguishing terminology related to electron configuration and orbitals. This carries over into their discussions where inappropriate terms are used synonymously (e.g., shell and orbital). This is not a new finding. Much of the misconception research being done (e.g., Griffiths et al., 1992; Howe, 1996; Osborne & Cosgrove, 1983) shows a very clear link between a weak descriptive language base and the logical development of science concepts.

Despite problems with configuration, the symbolic use of electron dot diagrams to indicate valence electrons seems relatively sound in this sample. If students have memorized the valence electron counting scheme as it relates to group number this becomes a trivial exercise. Pictorial representations beyond dot diagrams included primarily stick pictures and a very few students used wedge or Fisher-type conventions.

Most students represented orbitals as planar entities. The idea of a probability map in three-dimensional space has escaped many of these students. Whether this is because it was not a component of the instruction or lacked emphasis or appropriate modeling is unclear, however it forms the fundamental basis of bonding theories and therefore warrants adequate treatment by instructors. The exclusive use of textbook pictures for models can lead to misunderstandings on the part of the student. Many of the misconceptions evident in this survey may have conceivably arisen over the misapplication of the Bohr model or a planetary analogy. Use of analogies for the many abstractions of chemistry can be effective (Harrison & Treagust, 1994) but it is not uncommon for students to over-apply a familiar or poorly developed analogy. The advent of computer simulation may become a powerful tool for teachers in terms of developing better spatial perception skills in chemistry students.

Having had difficulty with the orbital concept in itself, it is not surprising that students were unable to label orbitals in simple bonding examples (HCl) much less understand the elevated concept of hybridization.

The VSEPR theory provides an excellent opportunity for teachers to improve students' spatial awareness. Teachers and students can build molecules in a very logical fashion without the use of algorithms or tables of lone pairs and bonding pairs. This survey demonstrated clearly that these rote approaches were relied upon in that students' answers included tabulated memory aids in the margin and unsubstantiated answers.

I prefer to use modeling clay, dowels and styrofoam balls in a discovery exercise. Students when asked how to separate four bonded styrofoam balls by the maximum angle will invariably say ninety degrees. The tetrahedron is then a good place to start. As the instructor removes a ball and leaves behind a delocalized lone pair (dowel) the trigonal pyramidal shape can be easily explained based on the number of electron pairs available. Removal of a second ball lends itself to an explanation of the v-shape followed by removal of the third ball to generate the linear molecule with two lone pairs. This approach encourages students to consider molecular shape in an intuitive way while taking into account the effects of repulsion of like charges, a simple concept. Though they can count bonding and lone pairs it doesn't form the basis for their understanding of the shape of the molecule.

Methane is a good example to introduce hybridization. An electron configuration can be built up quickly and the question presents itself; why doesn't carbon bond to two atoms? Some may guess that since methane exists, one of the 2s electrons must somehow be promoted to the 2p orbital. If then the teacher introduces the idea that experimentally all C-H bonds are equal in length, surely a 2p-1s bond will be different than a 2s-1s bond to hydrogen. This then develops the "need" for the hybridization concept. As offered by Grosslight et al. (1991) students must " . . . become more familiar with models as "testers" of interpretive frameworks . . . " The approach is intended to invoke disequilibrium (Saunders, 1992) in the students' concept, not dissimilar to what chemists may have experienced in trying to solve this problem years ago. Some may argue that there is no place for hybridization in high school chemistry curriculum. When the curriculum provides students with a glimpse of real science (Hawkins, 1965; Journet, 1994; Klapper, 1995;

Pizzini, Abell & Shepardson, 1988) it is worthwhile. VSEPR and hybridization concepts are unique examples of how chemists solve problems in a historical context; this makes them particularly valuable.

Conclusions

The work of Bent (1984) and Herron (1975) would suggest that many introductory chemistry students are at a concrete cognitive level which doesn't allow for a clear concept of such abstractions as electron configuration. The survey presented here provides evidence that students continue to have difficulty with seemingly rudimentry topics in chemistry. Though chemistry educators have known for some time that use of models can promote more effective conceptual learning, this study indicates that the impact is questionable. This may suggest that the method of model employment and perhaps as Beistel ,(1975) concludes, the ordering of chemistry topics is crucial (i.e., concrete to formal concepts). The students' need for concrete models in an effort to provide scaffolding for more formal quantum mechanical approaches may possibly be addressed by providing an hour glass approach. Curriculum designed around this strategy would allow students to firstly manipulate the generalized model, secondly deal with specifics or underpinnings of that model and finally extend and test the model. This approach as applied to chemistry instruction may involve students considering molecular shapes via physical models before the nature of bonding much less electrons is even addressed. This necessitates an instructional style which promotes "heads-on" rather than just hands-on.

If we hope to reach our chemistry students we must be ever cognizant of their cognitive strengths and attempt to diversify our discourse. In this isolated study what emerges is a lack of fundamental understanding of electronic behavior. Can we take the theoretical and make it more relevant in our instruction and assessment by asking students to draw, to build with models and to explain and test rather than dwell on lower level questioning which relies primarily on rote learning?

The language of chemistry is important and requires practice but the excitement for students lies in the reasoning and application. Making chemistry relevant and engaging means placing the student in the setting of the probing chemist, an emphasis on the process, solving problems, theorizing and constructing meaning for long-term understanding. Models are crucial to that aim and a great deal of energy should be invested in their appropriate use.

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